

Formation and local symmetry of Holstein polaron in t - J model

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The formation and local symmetry of spin-lattice polaron has been investigated semiclassically in the planar Holstein t - J -like models within the exact diagonalization method. Due to the interplay of strong correlations and electron-lattice interaction, the doped hole may either move freely or lead to the localized spin-lattice distortion and form a Holstein polaron. The formation of polaron breaks the translational symmetry by suppression of antiferromagnetic correlations and inducement of ferromagnetic correlations locally. Moreover, the breaking of local rotational symmetry around the polaron has been shown. The ground state is generically a parity singlet and the first excited state maybe a parity doublet. Further consequences of the density of states spectra for comparison with future STM experiments are discussed.

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Doping a Mott insulator has been regarded as the main physics in high T_c cuprate superconductors [1]. Single hole in the two-dimensional t - J model may form a ferromagnetic (FM) spin polaron for sufficiently small exchange coupling J [2]. For finite J , the distortion of the antiferromagnetic (AFM) background decays away from the hole and the competition between magnetic correlation and kinetic energy may result in the ground state with a spin polaron structure. This problem has been extensively investigated numerically [3–7]. To make a better comparison with angle-resolved photoemission spectroscopy (ARPES) experimental data, one need to include the nearest-neighboring (NN) and next-nearest-neighboring (NNN) hopping t' and t'' terms [8–10]. On the other hand, the role of electron-phonon (el -ph) coupling has gained much interest recently. One reason is that the ARPES data in doped metallic cuprates which showed the broadening of spectral lines at a certain momentum revealed the band dispersion renormalized by el -ph interaction [11, 12]. In addition, the interaction also shifts the energy of the states.

The doped charge carriers in the presence of both strong electronic correlations and electron-phonon interactions may lead to the formation of spin-lattice polaron. In particular, the AFM exchange interaction allows for spin flips leading to coherent hole motion at the bottom of the band and forms a spin polaron. In the presence of strong el -ph coupling, both the spin and lattice degrees of freedom become entangled and the spin polaron may transform into a spin-lattice polaron. The formation of this composite polaron may affect both the spin and lattice degrees of freedom locally. Recent ARPES experiments in undoped cuprates were interpreted in terms of strong el -ph coupling giving rise to localized polaron [11, 12]. The possibility of self-localization of holes in lightly doped cuprates has been studied [13]. It has been found that the effect of el -ph interaction on spin

polaron is strongly enhanced as compared to polaron in uncorrelated systems [14–19].

Recent atomically resolved scanning tunneling microscopy (STM) studies [20, 21] on strongly underdoped cuprates revealed a surprisingly pattern with the square symmetry of the lattice broken on a local scale. The origin of this broken local symmetry was attributed to the dopant impurity effect [22]. The broken symmetry states were shown to appear in the case of a hole confined to a cluster of sites centered at a impurity. Meanwhile the introduction of el -ph interaction to the t - J model may stabilize the half-doped stripes [23]. In the presence of strong el -ph coupling, the variations of hopping integral and spin-spin correlation around the impurity may become more remarkable and the composite spin-lattice polaron may show up.

In this paper, we shall discuss the formation of spin-lattice polaron and its relevance of local symmetry by investigating the Holstein t - J -like models with the exact diagonalization method. Due to the interplay of competing electronic correlations and el -ph interactions, the doped hole may either move through lattice freely or favor the composite spin-lattice polaron. The formation of Holstein polaron breaks the translational symmetry by suppression of AFM correlations and inducement of FM correlations locally. Moreover, the breaking of local rotational symmetry around the polaron center has been shown. The ground state is generically a parity singlet and the first excited state maybe a parity doublet. Further consequences of the tunneling spectra for comparison with future STM experiments will be discussed.

The two-dimensional single-band Holstein t - t' - J model

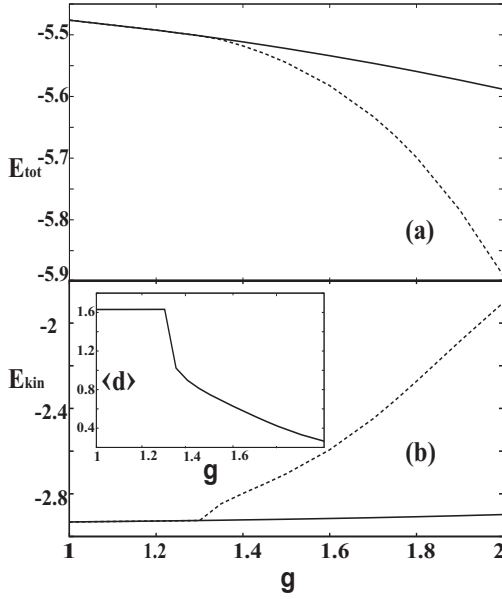


FIG. 1: The total energy (a) and kinetic energy (b) as a function of el -ph coupling constant g . The solid line corresponds to the delocalized state while the dashed line denotes the localized Holstein polaron state. The inset shows a measure of polaron size $\langle d \rangle$ as a function of g . We choose $t' = -0.1$ and $J = 0.3$.

in the adiabatic limit is defined by the Hamiltonian,

$$\mathcal{H} = -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - t' \sum_{\langle\langle i,j \rangle\rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - g \sum_i u_i n_i^h + \frac{K}{2} \sum_i u_i^2. \quad (1)$$

where $c_{i\sigma}^\dagger$ is an electron creation operator with spin σ at site i with a constraint of no double electron occupation due to strong electron correlations, \mathbf{S}_i is a spin operator for electron at site i , $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ refer to NN and NNN sites i and j . The first three terms in Eq. 1 represent the usual t - t' - J model Hamiltonian. The fourth term denotes the el -ph interaction. In the adiabatic limit, displacements u_i have been treated classically and determined by $u_i = g/K \langle n_i^h \rangle$. The hole density operator n_i^h is defined as $n_i^h = 1 - n_i = 1 - \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$. The last term is lattice elastic energy with elastic force constant K . The energy spectrum and eigenstates can be obtained through exact diagonalization method. The symmetry of the lowest energy state is sensitive to boundary condition and parameters. In our calculations, we choose $t = K = 1$, suitable for the cuprates, and adopt the periodic boundary condition.

Employed with the exact diagonalization method for a finite 16-site square cluster, the low-lying electronic states have been calculated as a function of el -ph coupling constant g . Due to the competition between electronic correlations and electron-lattice interactions, the

ground state has certain limiting cases. When g is very small, the ground state must correspond to a delocalized state, that is to say, doped hole may move through lattice freely so that the average occupation number of holes at each site is uniform. The presence of strong el -lattice interaction may clearly favor the localized hole state, which is a sliding periodic polaron lattice. Since we focus on the local properties of polaron, we use a very weak impurity to break the translational symmetry and pin down the sliding polaron lattice so that the doped single hole may stay around certain site. At $g \gg 1$ limit, the doped hole tends to be localized and results in large lattice distortion around that site. The corresponding ground state is a localized state with polaron formation. The evolution of total energy as well as kinetic energy of the system as a function of g is depicted in Fig. 1(a) and Fig. 1(b), respectively. The critical el -ph coupling $g_c \sim 1.3$ can be straightforwardly determined by distinguishing these two distinct states. Moreover we use the quantity $\langle d \rangle$ to measure the size of polaron qualitatively, $\langle d \rangle = \sum_i r_i \cdot n_i^h(r_i)$, where r_i is the distance between site i and polaron center. It is obvious that the larger $\langle d \rangle$ value may correspond to a larger polaron size. As shown in the inset of Fig. 1, as g increases, doped holes tend to concentrate at the polaron center so that the quantity $\langle d \rangle$ may be significantly suppressed. It is worth to mention that the critical point g_c is rather clearly revealed in the behaviors of $\langle d \rangle$ and kinetic energy than that of the total energy. Comparing with the previous study on the dopant impurity effect [22], the strong variations of hopping integral and spin-spin correlation around the polaron may lead to the formation of local lattice distortion and the appearance of tightly bounded spin-lattice polaron due to strong el -ph coupling [13].

Next we examine the effect of NNN hopping integral t' . As we know, the t' term plays an important role in understanding the superconducting correlations in cuprate superconductors [24–26]. In particular, the positive t' case corresponds to the electron-doped system while the negative t' case corresponds to the hole-doped system. In the following, we systematically study the dependence of g_c as a function of t' for two distinct t - J like models. Due to the competing tendency between the polaron formation with strong el -ph interaction and the itinerant electrons with large kinetic energy, we naturally expect that the formation of localized polaron may require stronger el -ph interaction to compensate larger kinetic energy $|t'|$ term. For the Holstein t - t' - J model, it is indeed the case as shown in Fig. 2(a) where g_c goes up as $|t'|$ increases. Another feature shown in Fig. 2(a) is the asymmetrical behavior between $t' < 0$ and $t' > 0$ regions. An intuitive physical understanding of such effect can be given as follows: for positive t' , the t' and t terms in kinetic energy match quite well, so that the positive t' term may enhance the kinetic energy more effective than the negative t' term, hence require stronger el -ph interaction g_c to realize the localization of Holstein polaron.

As suggested in recent studies, the t - t' - J - J' model may

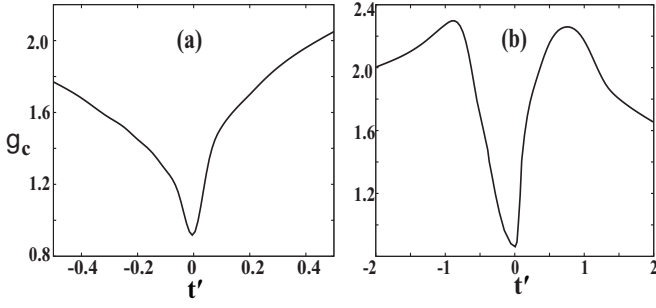


FIG. 2: The critical el -ph coupling g_c as a function of t' for Holstein t - t' - J model (a) and t - t' - J - J' model (b). We choose $J=0.3$ and $J'/J = (t'/t)^2$.

be suitable for iron-based superconductors [27, 28]. In such systems, the appropriate range of t' is much larger than that of cuprates and the NNN superexchange coupling is expressed as $J'/J = (t'/t)^2$. In the case of weak t' term, the results are similar to that of the Holstein t - t' - J model. The competing nature between J' term and J term may lead to the effect of geometrically frustration. In such systems, the pairwise J' interaction does not coincide with the square lattice geometry, which may suppress the NN AFM correlation functions. For stronger t' term as well as J' term, the suppression may become so strong that the local FM correlation may emerge around the polaron center. And it may result in the enhancement of kinetic energy and the reduction of the critical el -ph interaction g_c , which makes the formation of polaron easier. These relationships are clearly exhibited in Fig. 2(b) where g_c decreases as t' becomes quite large.

Similar to the dopant impurity case [22], the presence of a localized spin-lattice polaron may affect not only the local charge and local spin distributions but also the symmetry of the ground state wavefunction. In the following, we adopt the same parity symmetry to characterize different quantum states [22]. In particular, we focus on the reflection symmetries of a two-dimensional square lattice with respect to x - and y -axes passing through the center of polaron (P_x and P_y respectively) and on the parity $P_x P_y$. Since $[P_{x(y)}, H] = 0$, we may classify states according to the quantum numbers of P_x , P_y . We denote the state with $(P_x = +1, P_y = +1)$ as state $(++)$, doubly degenerate state $(+1, -1)$, and $(-1, +1)$ as states $(+-)$ and $(-+)$, and $(-1, -1)$ as state $(--)$. As we know, in the absence of el -ph interactions, for a 16 - (4×4) site cluster with periodic boundary condition, the ground state of a single hole in the t - t' - J model has a four-fold symmetry for $t' < 0$, which can be represented by their parity symmetry $(++)$, $(+-)$, $(-+)$, $(--)$.

As clearly shown in Fig. 3, the ground states have 4-fold degeneracies for weak el -ph interaction $g < g_c \sim 1.3$. For g becomes slightly larger than g_c , such degeneracies are broken. We note that the four low-lying states with different reflection symmetries are quite close in energy. The state with $(++)$ symmetry always has the lowest en-

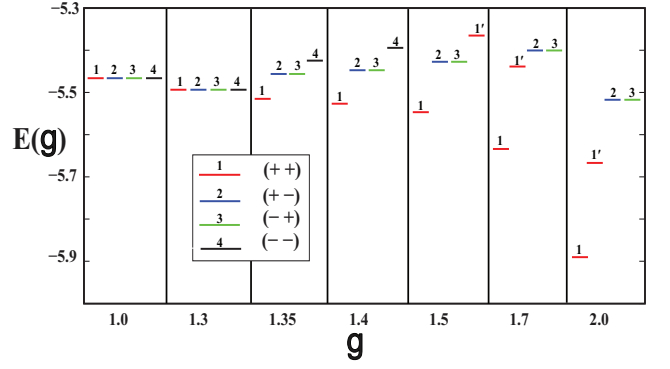


FIG. 3: (Color online) Evolution of four low-lying energy levels and their corresponding parity symmetries as a function of el -ph coupling g . We choose $t' = -0.1$ and $J = 0.3$.

ergy, the doubly degenerated states with parity symmetry $(+-)$ and $(-+)$ correspond to the first excited states, while the state with $(--)$ symmetry is the second excited state. As g exceeds 1.5, the state $(++)$ originally at much higher energy may drop down significantly and cross the singly degenerated $(--)$ state. For $g > 1.7$, both two lowest energy states have the $(++)$ symmetry. According to our numerical results, the ground state of spin-lattice polaron is quite robust in the $(++)$ symmetry.

To explore further the interplay between spin and charge degrees of freedom, we study the spatial distribution of spin-spin correlation function and hopping integral around the polaron. As depicted in Table I, we show the expectation value of spin-spin correlation function $\langle S_i S_j \rangle$ as well as hopping integral $\langle c_i^\dagger c_j \rangle$ for six distinct bonds illustrated in Fig. 4(a). The interplay of strong correlation and el -ph interaction may lead to hole localization and result in a remarkable hopping integral and a weak FM spin-spin correlation function around the hole. In particular, the AFM correlation along bond 1 is completely suppressed, and a weak FM correlation emerges. The spin-spin correlation function recovers quickly to the value -0.34 for farther bonds. Meanwhile the hopping integral along bond 1 is much stronger than that of the rest bonds and the hopping integral vanishes quickly close to the lattice boundary. It is rather clear that the inducement of local FM correlations around the polaron may help the hole moving around more efficiently, then maximizing the local kinetic energy. Hence the mutual cooperative effect between spin and lattice degrees of freedom has been clearly revealed. For Holstein t - J model in infinite dimensions, the interplay between the formation of a lattice and magnetic polaron in the case of a single hole in the AFM background has been studied before [29]. It shows that the presence of AFM correlations favors the formation of the lattice polaron at lower values of the el -ph coupling. Our numerical calculations agree well with their results.

Furthermore, we investigate the parameter dependence

TABLE I: The spin-spin correlation functions and hopping integrals for various bonds in a 16-site cluster with periodic boundary condition at $t' = -0.1$, $J = 0.3$ and $g = 2.0$. The bond indices are labeled in Fig. 4(a).

bond index	1	2	3	4	5	6
$-\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$	-0.034	0.335	0.342	0.337	0.346	0.347
$\langle c_i^\dagger c_j \rangle$	0.405	0.018	0.021	0.002	0.002	0.000

of the spin-spin correlation function for both t - t' - J model and t - t' - J - J' model. For these two models, the spin-spin correlation function on bond 1 and bond 2 shows quite different behaviors. For t - t' - J model, there is always large AFM correlation on bond 2, while weak AFM or FM correlation shows up on bond 1. This strong suppression of AFM correlation locally around the center of polaron is due to the dramatic lattice distortion or the polaron formation. However, such strong suppression of AFM correlation on bond 2 may be significantly modified in t - t' - J - J' model for large t' case. In such case, the introduction of large t' may lead to the enhancement of kinetic energy and the strong frustration effect due to J' term may greatly suppress the AFM correlation on bond 2. Meanwhile the size of the spin-lattice polaron may be enlarged.

To understand the nature of states with different parity symmetries, the spatial distribution of S_z has been calculated and illustrated in Fig. 4. For delocalized states, as shown in Fig. 4(b)-4(e), states with four distinct parity symmetry $(++)$, $(+-)$, $(-+)$, $(--)$ for t - t' - J model dis-

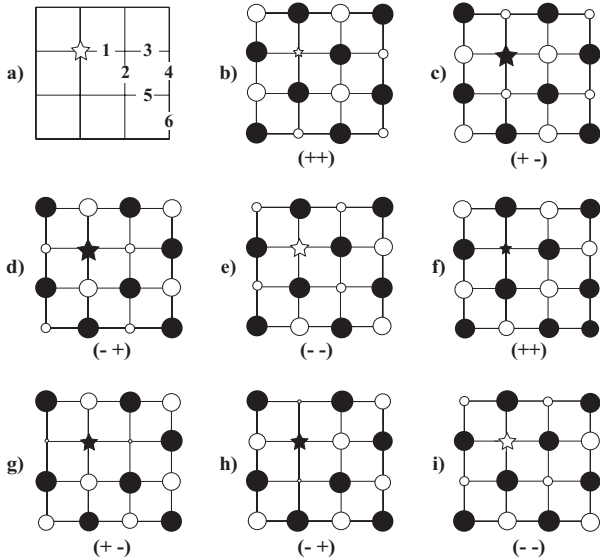


FIG. 4: The spatial distribution of S_z for t - t' - J model. Delocalized states are shown in figure (b)-(e) for different parity symmetries. Localized states are shown in figure (f)-(i). The diameter of each circle is proportional to the value of local $|S_z|$. White (Black) circle represents up (down) spin. The star symbol labels the center of polaron.

play quite different patterns. In Fig. 4(b), for state with $(++)$ symmetry, weak up spin appears at the polaron center while weak AFM correlation shows up between the polaron center and its four nearest neighbors. In Fig. 4(c)-(d), for states with $(+-)$ and $(-+)$ symmetry, the asymmetry between two neighboring sites of polaron center along x and y directions is clearly shown. For localized states, the spatial distribution of S_z patterns are shown in Fig. 4(f)-4(i), respectively, corresponding to different symmetry states. For $(++)$ symmetry state, weak down spin appears at the polaron center while weak FM correlation shows up between the polaron center and its four nearest neighbors. As we know, the doped hole may concentrate at the polaron center where the weak FM correlation may emerge. It is obvious that this $(++)$ symmetry state is energetically favorable to the spin-lattice polaron formation. In Fig. 4(g)-(h), the asymmetry between two neighboring sites of polaron center along x and y directions becomes more significant than the delocalized states. Of all four parity symmetry states, this $(++)$ symmetry state has the lowest energy. In addition, we checked the spatial distribution of S_z in t - t' - J - J' model and similar results are obtained. In both cases, the ground state of spin-lattice polaron prefers the $(++)$ parity symmetry.

In order to check the existence of spin-lattice polaron, integrated differential conductance as a function of cutoff voltage is calculated to be compared with future STM experiments. Following the STM tunneling theory [30], we write the integrated current at \mathbf{r} up to a positive voltage V as

$$I(\mathbf{r}, \omega) \propto \sum_{\sigma, m} |\langle m | a_{\mathbf{r}, \sigma}^\dagger | \psi^{1h} \rangle|^2 \theta(\omega - E_m + E^{1h}). \quad (2)$$

where $a_{\mathbf{r}, \sigma}^\dagger$ is the electron creation operator with spin σ at site \mathbf{r} , $|m\rangle$ are eigenstates of the half-filled system with energy E_m , $\omega = eV$, and θ is a step function. The $|\psi^{1h}\rangle$ denotes the single-hole eigenstate with energy E^{1h} . In the following, we show the I - ω curve on various sites and for different el -ph coupling g . For convenience, we shift the origin of x -axis by $\omega_0 = \omega + \omega_{ex}$ where $\omega_{ex} = E_0 - E_0^{1h}$ and E_0 , E_0^{1h} correspond to the ground state of half-filled system and single-hole system, respectively. Here we consider the contributions from low-lying energy states of the single-hole system.

As we know already, the doped hole tends to stay around the polaron center and the hole density at the polaron center is more significant than that of on other sites by increasing the el -ph interaction g . Thus we expect the integrated current at the polaron center would become larger when g goes up. This result is clearly shown in the left panel of Fig. 5. In the case of impurity doped cuprates, the conductance pattern is anisotropic as the tip of a tunneling microscope scans above the Cu-O-Cu bonds along the $x(y)$ -axes. This anisotropy is quite pronounced at voltage around $\omega \sim J$. In the present case, due to the formation of spin-lattice polaron, the ground state of one-hole system has $(++)$ symmetry, the first excited

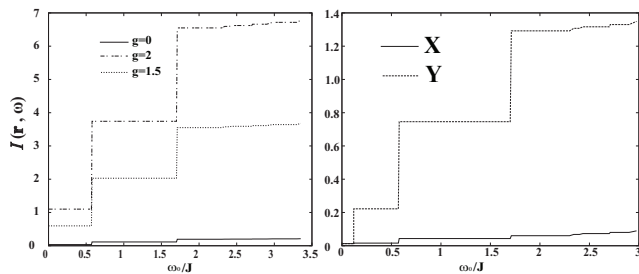


FIG. 5: The local integrated current up to voltage V for different sites at various e -ph coupling constant g as a function of ω . The left panel shows the results for signal at the center of polaron for different g values. The right panel depicts the results for signal at the two NN sites respectively along x and y directions.

state corresponds to the doubly degenerated states $(+-)$ and $(-+)$. The presence of quadrupole interaction of two single-hole states or by other couplings may not change the symmetry of ground state but may destroy the two-fold degeneracy of first excited state. We consider the system to be in one of the two degenerate states, say in the state of $(+-)$. As depicted in the right panel of Fig. 5, below certain cutoff-energy ($\sim 0.11J$), the integrated current shows four-fold rotational symmetry for the state with $(++)$ symmetry. For the higher cutoff-energy, the first excited state with $(+-)$ symmetry may play important role in the local symmetry breaking for the signals along x and y - directions.

Our numerical results can be qualitatively understood in terms of the renormalized mean-field method for t - J model. Due to the presence of spatial inhomogeneous polaron, the renormalized factor g_t and g_s become site-dependent. According to previous study [31], the renormalized factor of kinetic energy on the bond connecting two sites i and j can be expressed as $g_t^{ij} \sim \sqrt{\delta_i \delta_j}$. As we know, in the case of strong el -ph interaction, the hole

density is highly localized at the center of Holstein polaron. It is obvious that the bonds with appreciable hopping integral show up only around the polaron and may result in the suppression of AFM correlation locally. For the delocalized states, g_t^{ij} is simply a constant and so is the AFM correlation function. The above qualitative analysis agrees reasonable well with our numerical results shown in Fig. 3 and Table.I.

In summary, we study both the formation and local symmetry of spin-lattice polaron semiclassically in the planar Holstein t - J -like models within the exact diagonalization method. Due to the interplay of competing interactions among electronic correlations and el -phonon interactions, the doped hole may either move freely or lead to the localized spin-lattice distortion and form a Holstein polaron. Since the formation of polaron breaks the translational symmetry, we use the parity symmetry with respect to the polaron center to characterize the localized states. The presence of spin-lattice polaron may suppress the AFM correlations and induce the FM correlations locally around the polaron. This effect may further stabilize the spin-lattice polaron. Moreover, this affect may lead to a strong localized state with $(++)$ parity symmetry as ground state. Moreover, the breaking of local rotational symmetry around the polaron has been shown for certain voltage cutoff. The present investigation on the polaron formation and local symmetry may provide useful information for future STM experimental tests.

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